



# Full wwPDB X-ray Structure Validation Report i

Oct 4, 2023 – 07:22 PM EDT

PDB ID : 6TZT  
Title : Crystal structure of human alpha/epsilon-COP of the COPI vesicular coat bound to alpha-COP STM2  
Authors : Travis, S.M.; Hughson, F.M.  
Deposited on : 2019-08-13  
Resolution : 3.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

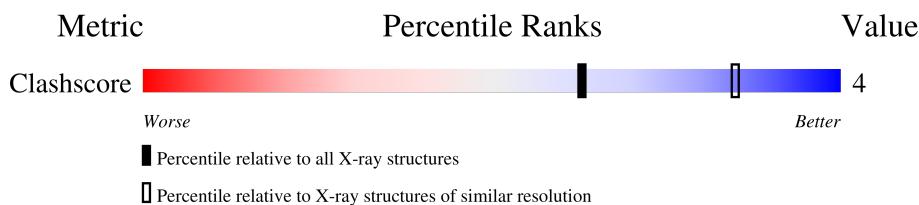
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 Å.

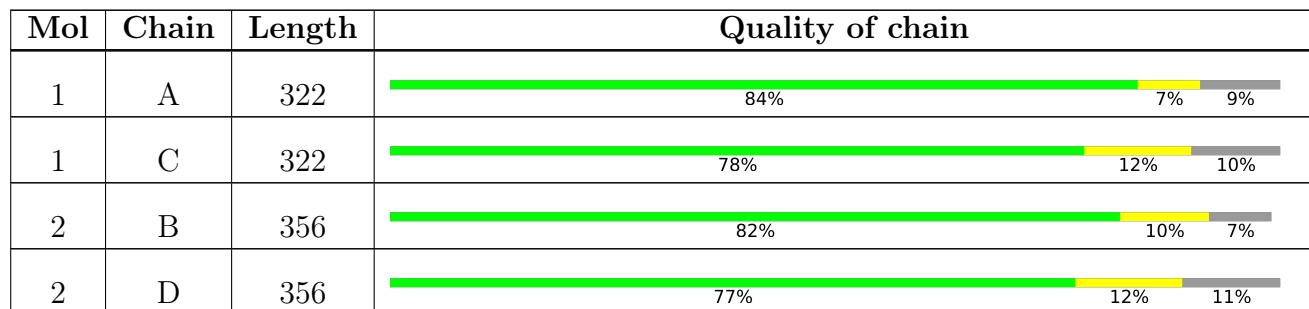
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1864 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.



## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9801 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2332	1466	404	451	11	0	1	0
1	C	290	2320	1458	403	448	11	0	1	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP O14579
A	-12	GLY	-	expression tag	UNP O14579
A	-11	SER	-	expression tag	UNP O14579
A	-10	SER	-	expression tag	UNP O14579
A	-9	HIS	-	expression tag	UNP O14579
A	-8	HIS	-	expression tag	UNP O14579
A	-7	HIS	-	expression tag	UNP O14579
A	-6	HIS	-	expression tag	UNP O14579
A	-5	HIS	-	expression tag	UNP O14579
A	-4	HIS	-	expression tag	UNP O14579
A	-3	SER	-	expression tag	UNP O14579
A	-2	GLN	-	expression tag	UNP O14579
A	-1	ASP	-	expression tag	UNP O14579
A	0	PRO	-	expression tag	UNP O14579
C	-13	MET	-	expression tag	UNP O14579
C	-12	GLY	-	expression tag	UNP O14579
C	-11	SER	-	expression tag	UNP O14579
C	-10	SER	-	expression tag	UNP O14579
C	-9	HIS	-	expression tag	UNP O14579
C	-8	HIS	-	expression tag	UNP O14579
C	-7	HIS	-	expression tag	UNP O14579
C	-6	HIS	-	expression tag	UNP O14579
C	-5	HIS	-	expression tag	UNP O14579
C	-4	HIS	-	expression tag	UNP O14579
C	-3	SER	-	expression tag	UNP O14579

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLN	-	expression tag	UNP O14579
C	-1	ASP	-	expression tag	UNP O14579
C	0	PRO	-	expression tag	UNP O14579

- Molecule 2 is a protein called Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2624	1684	453	472	15			
2	D	318	Total	C	N	O	S	0	0	0
			2524	1619	437	453	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	869	MET	-	expression tag	UNP P53621
D	869	MET	-	expression tag	UNP P53621

- Molecule 3 is water.

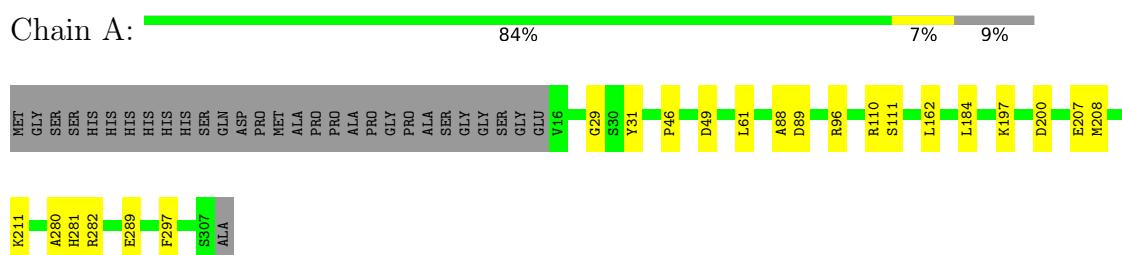
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0

### 3 Residue-property plots

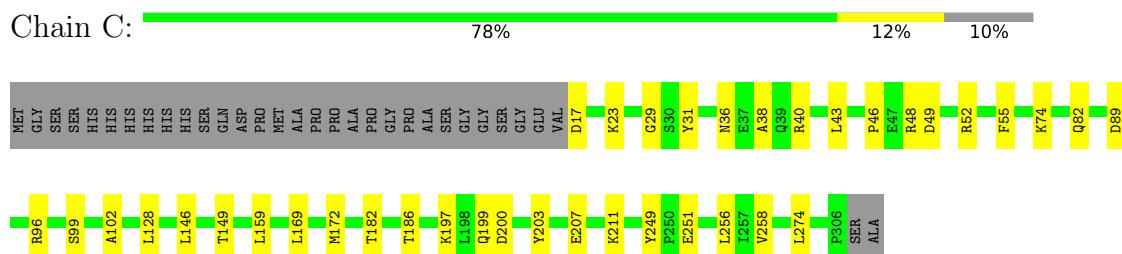
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

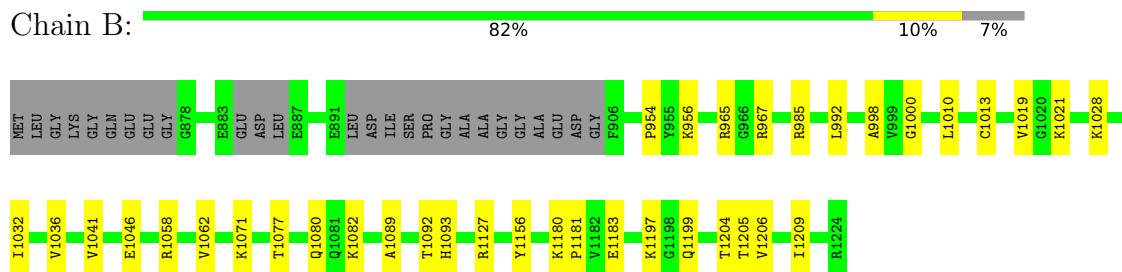
- Molecule 1: Coatomer subunit epsilon



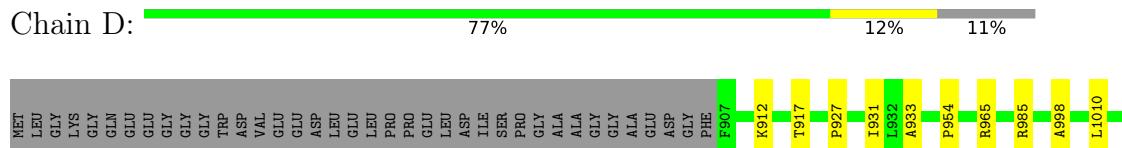
- Molecule 1: Coatomer subunit epsilon



- Molecule 2: Coatomer subunit alpha



- Molecule 2: Coatomer subunit alpha





## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.47 Å    138.47 Å    192.87 Å 90.00°    90.00°    120.00°	Depositor
Resolution (Å)	29.62 – 3.06	Depositor
% Data completeness (in resolution range)	99.8 (29.62-3.06)	Depositor
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.28 (at 3.06 Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R <sub>free</sub>	0.178 , 0.223	Depositor
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtriage
Anisotropy	0.044	Xtriage
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.51	0/2376	0.65	0/3216
1	C	0.43	0/2364	0.63	0/3200
2	B	0.50	0/2682	0.66	0/3634
2	D	0.45	0/2579	0.64	0/3497
All	All	0.47	0/10001	0.65	0/13547

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2332	0	2297	14	0
1	C	2320	0	2287	23	0
2	B	2624	0	2670	23	0
2	D	2524	0	2584	30	0
3	B	1	0	0	1	0
All	All	9801	0	9838	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1204:THR:HG22	2:D:1206:VAL:H	1.35	0.91
2:B:954:PRO:HG2	2:B:1206:VAL:HG12	1.53	0.89
2:D:954:PRO:HG2	2:D:1206:VAL:HG12	1.55	0.88
2:D:1092:THR:HG23	2:D:1127:ARG:HH12	1.39	0.87
2:B:1183:GLU:HG3	2:B:1197:LYS:HB2	1.67	0.77
1:C:89:ASP:OD2	1:C:96:ARG:NH1	2.20	0.74
1:A:289:GLU:OE1	2:B:967:ARG:NH2	2.21	0.73
1:C:46:PRO:HA	1:C:49:ASP:HB2	1.76	0.66
1:C:23:LYS:HG2	1:C:55:PHE:CE2	2.31	0.64
2:D:1077:THR:HB	2:D:1080:GLN:H	1.65	0.62
2:B:1013:CYS:SG	2:B:1028:LYS:HB3	2.40	0.61
2:D:985:ARG:HB3	2:D:998:ALA:HA	1.81	0.61
1:C:17:ASP:OD1	1:C:48:ARG:NH1	2.33	0.61
1:A:89:ASP:OD2	1:A:96:ARG:NH1	2.35	0.59
2:D:1204:THR:HG21	2:D:1207:THR:HG23	1.84	0.59
1:A:207:GLU:HG2	1:A:211:LYS:HE2	1.85	0.59
2:B:965:ARG:NE	2:B:1000:GLY:HA3	2.17	0.59
2:B:1092:THR:HG23	2:B:1127:ARG:HH22	1.67	0.59
2:D:1183:GLU:HG3	2:D:1197:LYS:HB2	1.85	0.59
1:C:199:GLN:HG3	1:C:203:TYR:CE2	2.38	0.59
1:A:61:LEU:HD21	1:A:88:ALA:HB2	1.86	0.57
1:C:172:MET:HG3	1:C:182:THR:HG23	1.86	0.57
2:D:1090:TYR:CZ	2:D:1175:PRO:HD3	2.38	0.57
2:D:1092:THR:HG22	2:D:1093:HIS:ND1	2.21	0.56
2:B:1058:ARG:O	2:B:1062:VAL:HG13	2.07	0.55
1:A:207:GLU:O	1:A:211:LYS:HG2	2.07	0.54
1:A:184:LEU:HD21	1:A:208:MET:HE3	1.90	0.54
1:C:36:ASN:O	1:C:40:ARG:HG2	2.08	0.53
2:D:1176:ILE:HG21	2:D:1182:VAL:HG12	1.90	0.53
1:C:197:LYS:O	1:C:200:ASP:HB2	2.10	0.52
2:B:1089:ALA:O	2:B:1092:THR:HB	2.10	0.51
2:B:1092:THR:HG22	2:B:1093:HIS:HD2	1.76	0.51
1:C:43:LEU:HD21	1:C:52:ARG:NH1	2.26	0.50
1:C:74:LYS:O	1:C:82:GLN:NE2	2.41	0.50
2:B:1019:VAL:HG13	2:B:1021:LYS:HG3	1.93	0.50
2:B:1082:LYS:HE2	2:B:1156:TYR:HB3	1.93	0.50
2:B:1077:THR:HB	2:B:1080:GLN:H	1.78	0.48
2:D:1130:GLU:O	2:D:1130:GLU:HG2	2.13	0.48
2:D:1204:THR:HG23	2:D:1206:VAL:HG22	1.96	0.48
1:A:281:HIS:CD2	1:A:282:ARG:HE	2.32	0.48
1:C:159:LEU:HD22	2:D:912:LYS:HG2	1.96	0.48
2:B:1041:VAL:HG13	2:B:1046:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:O	1:A:111:SER:HB3	2.14	0.47
1:A:197:LYS:O	1:A:200:ASP:HB2	2.14	0.47
2:B:1180:LYS:HB3	2:B:1181:PRO:HD2	1.96	0.46
1:A:280:ALA:O	1:A:282:ARG:HG2	2.15	0.46
2:D:1204:THR:CG2	2:D:1206:VAL:HG22	2.45	0.46
1:C:38:ALA:O	1:C:52:ARG:HD2	2.15	0.46
2:B:1092:THR:HG23	2:B:1127:ARG:NH2	2.31	0.46
2:D:1176:ILE:HG21	2:D:1182:VAL:CG1	2.46	0.46
2:D:927:PRO:O	2:D:931:ILE:HG13	2.17	0.45
1:C:29:GLY:HA2	1:C:31:TYR:CE1	2.52	0.45
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.74	0.45
1:C:169:LEU:HD21	1:C:186:THR:HG22	1.99	0.45
2:D:1010:LEU:HD12	2:D:1010:LEU:HA	1.71	0.45
1:C:207:GLU:O	1:C:211:LYS:HG2	2.16	0.44
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.71	0.44
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.82	0.44
2:B:985:ARG:HB3	2:B:998:ALA:HA	1.98	0.44
1:C:99:SER:O	1:C:102:ALA:HB3	2.18	0.44
2:D:1089:ALA:O	2:D:1092:THR:HB	2.18	0.44
2:B:1032:ILE:O	2:B:1036:VAL:HG23	2.18	0.43
2:D:1016:LEU:HD23	2:D:1016:LEU:HA	1.81	0.43
1:C:146:LEU:HD11	1:C:172:MET:HB2	2.01	0.43
2:B:1204:THR:O	2:B:1205:THR:HG22	2.18	0.43
1:C:274:LEU:HD12	1:C:274:LEU:HA	1.78	0.43
2:D:1180:LYS:HB3	2:D:1181:PRO:HD2	2.01	0.43
2:D:1019:VAL:HG13	2:D:1021:LYS:HG3	2.01	0.42
2:D:1083:ARG:O	2:D:1087:MET:HG3	2.19	0.42
2:B:1199:GLN:O	2:B:1209:ILE:HG13	2.19	0.42
2:D:1101:MET:HA	2:D:1104:VAL:HG13	2.00	0.42
1:A:46:PRO:HA	1:A:49:ASP:HB2	2.00	0.42
1:A:162:LEU:HD23	2:B:992:LEU:HD21	2.01	0.42
2:B:1071:LYS:NZ	3:B:1301:HOH:O	2.53	0.42
2:D:917:THR:HB	2:D:933:ALA:HB1	2.02	0.41
2:D:1013:CYS:HB3	2:D:1029:PHE:CZ	2.54	0.41
2:D:1058:ARG:HD2	2:D:1190:ALA:HA	2.03	0.41
1:A:29:GLY:HA2	1:A:31:TYR:CE1	2.55	0.41
1:C:258:VAL:HG22	2:D:965:ARG:HA	2.01	0.41
1:C:149:THR:HB	1:C:172:MET:HE1	2.02	0.41
2:D:1041:VAL:HG13	2:D:1046:GLU:HB2	2.02	0.41
1:A:297:PHE:CD2	2:B:956:LYS:HG3	2.56	0.41
1:C:249:TYR:CE2	1:C:251:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1013:CYS:SG	2:D:1028:LYS:HB3	2.61	0.41
2:D:1102:ILE:HG23	2:D:1128:LEU:HD13	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [\(i\)](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section is therefore empty.